

# Inelastic electron transport in polymer nanofibers

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In this paper we present theoretical analysis of the electron transport in conducting polymers being in a metal-like state. We concentrate on the study of the effects of temperature on characteristics of the transport. We treat a conducting polymer in the metal state as a network of metallic-like grains embedded in poorly conducting environment which consists of randomly distributed polymeric chains. We carry out the present studies assuming that the intergrain conduction is mostly provided by electron quantum tunneling via intermediate states localized on polymer chains between the grains. To analyze the effects of temperature on this kind of electron intergrain transport we represent the thermal environment as a phonon bath coupled to the intermediate state. The electron transmission is computed using the Buttiker model within the scattering matrix formalism. This approach is further developed, and the dephasing parameter is expressed in terms of relevant energies including the thermal energy. It is shown that temperature dependencies of both current and conductance associated with the above transport mechanism differ from those typical for other conduction mechanisms in conducting polymers. This could be useful to separate out the contribution from the intergrain electron tunneling to the net electric current in transport experiments on various polymer nanofibers. The proposed model could be used to analyze inelastic electron transport through molecular junctions.

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## I. INTRODUCTION

At present, electronic transport properties of conducting polymers such as doped polyacetylen and polyaniline-polyethylene oxides attract an intense interest and attention of the research community [1, 2]. These materials, as well as carbon nanotubes, are expected to have various applications in fabrication of nanodevices. Significant efforts have been applied to study conduction mechanisms in the polymers. This is a rather complex topic for electron transport in conducting polymers shows both metallic and non-metallic features, and various transport mechanisms contribute to the resulting pattern.

An important contribution to the conduction in these substances is provided by the phonon assisted electron hopping between the conducting islands or variable range hopping between localized electronic states [2, 3]. The effect of these transport mechanisms strongly depends on the intensity of stochastic nuclear motions. The latter increases as temperature rises, and this brings a significant enhancement of the corresponding contribution to the conductivity. The temperature dependence of the “hopping” conductivity  $\sigma(T)$  is given by the Mott’s expression [4]:

$$\sigma(T) = \sigma(0) \exp[-(T_0/T)^p] \quad (1)$$

where  $T_0$  is the characteristic temperature of a particular material, and the parameter  $p$  takes on values 0.25, 0.33 or 0.5 depending on the dimensions of the hopping processes. Also, it was proposed that phonon-assisted transport in low-dimensional structures such as nanofibers and nanotubes may be substantially in-

fluenced due to electron interactions [5, 6]. This results in the power-low temperature dependencies of the conductance  $G(T)$  at low values of the bias voltage  $V$  ( $eV < kT$ ,  $k$  being the Boltzmann constant), namely:  $G \sim T^\alpha$ . Experimental data for the conductance of some nanofibers and nanotubes match this power-low reasonably well, bearing in mind that the value of the exponent  $\alpha$  varies within a broad range. For instance,  $\alpha$  was reported to accept values about 0.35 for carbon nanotubes [7], and  $\alpha \sim 2.2 \div 7.2$  for various polyacetylene nanofibers [8, 9].

In general, hopping transport mechanism is very important in disordered materials with localized states. For this kind of transport phonons play part of a source of electrical conductivity. Accordingly, the hopping contribution to the conductivity always increases as temperature rises, and more available phonons appear. When polymers are in the insulating state, the hopping transport mechanism predominates and determines the temperature dependencies of transport characteristics.

In metallic state of conducting polymers free charge carriers appear, and their motion strongly contributes to the conductance. While moving, the charge carriers undergo scattering by phonons and impurities. This results in the conductivity stepping down. Metallic-like features in the temperature dependencies of dc conductivity of some polymeric materials and carbon nanotubes were repeatedly reported. For instance, the decrease in the conductivity upon heating was observed in polyaniline nanofibers Refs. [10, 11] and carbon nanotubes [12]. However, this electron diffusion is not the only transport mechanism in the metallic state. The con-

ducting polymers could be described as granular metals, where conducting metallic-like islands (grains) made out of densely packed polymer chains are embedded in the amorphous poorly conducting environment where the chains are disorderly arranged [1]. Prigodin and Epstein suggested that the electron transport between metallic islands mostly occurs as a result of electron resonance tunneling through intermediate states localized on the polymer chains in between the grains [13]. The effect of phonons on this kind of electron transport may be very significant. These phonons bring an inelastic component to the intergrain current and underline the interplay between the transport by the electron tunneling and the thermally assisted dissipative transport. Also, they may cause some other effects, as was shown while developing the theory of conduction through the molecules [14, 15, 16, 17].

Here, we concentrate on the analysis of temperature dependencies of the electric current and conductance associated with the resonance tunneling transport mechanism. The analysis is motivated by an assumption that various conduction mechanisms may simultaneously contribute to the charge transport in conducting polymers, and their relative effects could significantly differ depending on the specifics of synthesis and processing of polymeric materials. The temperature dependencies of the resulting transport characteristics may help to identify the predominating transport mechanism for a particular sample under particular conditions, providing a deeper insight in the nature of electron transport in conducting polymers.

The issue is of particular importance because the relevant transport experiments are often implemented at room temperature (see e.g. [18]), so that the influence of phonons cannot be disregarded. Therefore we study the effect of temperature (stochastic nuclear motions) on the resonance electron tunneling between metalliclike grains (islands) in polymer nanofibers. We apply the obtained results to analyze electron transport in conducting polymers. However, these results could be easily adapted to study some phonon induced effects in the electron transport through metal-molecule junctions and other kinds of quantum dots coupled to the source and drain reservoirs.

## II. MODEL AND RESULTS

The transmission coefficient for the electron intergrain resonance tunneling is determined with the probability of finding the resonance state. The latter is estimated as  $P \sim \exp(-L/\xi)$  ( $L$  is the average distance between the adjacent grains, and  $\xi$  is the localization length for electrons), and takes values much smaller than unity but much greater than the transmission probability for sequential hoppings along the chains,  $P_h \sim \exp(-2L/\xi)$  [19]. The probability for existence of a resonance state

at a certain chain is rather low, so only a few out of the whole set of the chains connecting two grains are participating in the process of intergrain electron transport. Therefore one could assume that any two metallic domains are connected by a single chain providing an intermediate state for the resonance tunneling. All remaining chains can be neglected for they poorly contribute to the transport compared to the resonance chain. Within this approach the intergrain conduction strongly resembles the electron conduction through a molecular bridge connecting two metallic leads, and similar formalism could be employed to compute it.

Correspondingly, in calculations of the current we employ the formula which describes the electronic transport through a junction including two leads (adjacent grains) and the intermediate state coupled to them. We treat the grains as free electron reservoirs in thermal equilibrium. This assumption is justified when the intermediate state (the bridge) is weakly coupled to the leads and conduction is much smaller than the quantum conductance  $G_0 = 2e^2/h$  ( $e, h$  are the electron charge, and the Planck constant, respectively). Due to the low probabilities for the resonance tunneling between the metallic islands in the conducting polymers the above assumption may be considered as a reasonable one. So, we can employ the well-known expression for the electron current through the junction [20], and we write:

$$I = \frac{2en}{h} \int_{-\infty}^{\infty} dE T(E) [f_1(E) - f_2(E)]. \quad (2)$$

Here,  $n$  is the number of the working channels in the fiber,  $f_{1,2}(E)$  are Fermi functions taken with the different contact chemical potentials  $\mu_{1,2}$  for the grains. The chemical potentials differ due to the bias voltage  $\Delta V$  applied across the grains:

$$\mu_1 = E_F + (1 - \eta)e\Delta V; \quad \mu_2 = E_F - \eta e\Delta V. \quad (3)$$

The parameter  $\eta$  characterizes how the voltage  $\Delta V$  is divided between the grains;  $E_F$  is the equilibrium Fermi energy of the system including the pair of grains and the resonance chain in between, and  $T(E)$  is the electron transmission function.

Realistic polymer nanofibers have diameters within the range  $20 \div 100$  nm, and lengths of the order of a few microns. This is much greater than the typical size of both metallic-like grains and intergrain separations which take on values  $\sim 5 \div 10$  nm (see e.g. [18, 21]). Therefore, we may treat a nanofiber as a set of working channels connected in parallel, any single channel being a sequence of grains connected with the resonance polymer chains. The net current in the fiber is the sum of currents flowing in these channels, and the voltage  $V$  applied across the whole fiber is distributed among sequential pairs of grains along a single channel. So, the voltage  $\Delta V$  applied across two adjacent grains could be roughly esti-

mated as  $\Delta V \sim VL/L_0$  where  $L$  is the average separation between the grains, and  $L_0$  is the fiber length. In realistic fibers the ratio  $\Delta V/V$  may take on values of the order of  $10^{-2} \div 10^{-3}$ .

To proceed we must compute  $T(E)$ . An important issue in calculation of the transmission is the effect of stochastic nuclear motions in the environment of the resonance state. When the dissipation is strong (e.g. within the strong thermal coupling limit), the inelastic (hopping) contribution to the intergrain current predominates, replacing the coherent tunneling dominating at weak dephasing. Typically, at room temperatures the intergrain electron transport in conducting polymers occurs within an intermediate regime, when both coherent and incoherent contributions to the electron transmission are manifested.

The general approach to the electron transport studies in the presence of dissipation is the reduced dynamics density-matrix formalism (see, e.g., Refs. [22] and [23]). This microscopic computational approach has the advantages of being capable of providing the detailed dynamics information. However, this information is usually more redundant than necessary, as far as standard transport experiments in conducting polymer nanofibers are concerned. There exists an alternative approach using the scattering-matrix formalism and the phenomenological Buttiker dephasing model [24, 25]. Adopting this phenomenological model we are able to analytically treat the problem, and the results agree with those obtained by means of more sophisticated computational methods, as was demonstrated in the earlier work [14]. However, this alternative approach has some significant shortcomings. Its main disadvantage is that the dissipative effects are described in terms of a phenomenological dephasing parameter  $\epsilon$  whose dependence of the characteristic factors affecting the transport (such as the temperature, the electron-phonon coupling strength and some others) remains unclear. Here, we carry out our analysis within the framework of the phenomenological Buttiker's dephasing model but we modify the latter to elucidate the relation of the dephasing parameter  $\epsilon$  to the relevant energies characterizing the electron transport in the considered system.

In studies of the intergrain electron transport in conducting polymers the "bridge" between two grains inserts a single electron state. Therefore we may treat the electron transport as a combination of tunneling through two barriers (the first one separates the left metallic domain from the intermediate state in the middle of the resonance chain, and the second separates this state from the right grain, supposing the transport is from the left to the right) affected by inelastic scattering at the bridge, as shown in the Fig. 1. The barriers are represented by the squares, and the triangle in between imitates a scatterer coupling the bridge to a dissipative electron reservoir.

An electron could be injected into this system, and/or

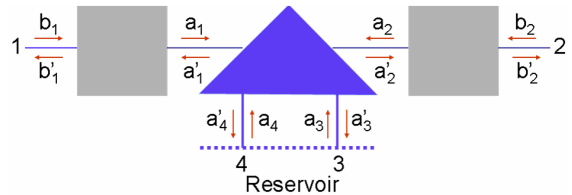


FIG. 1: Schematic drawing illustrating the intergrain electron transport in the presence of dissipation [24].

leave from there via four channels indicated in this Figure. Incoming particle fluxes ( $J_i$ ) are related to those outgoing from the system ( $J'_j$ ) by means of the transmission matrix  $T$ , [24, 25]

$$J'_j = \sum_i T_{ji} J_i, \quad 1 \leq i, j \leq 4. \quad (4)$$

Off-diagonal matrix elements  $T_{ji}(E)$  are probabilities for the electron to be transmitted from the channel  $i$  to the channel  $j$ , whereas diagonal matrix elements  $T_{ii}(E)$  are probabilities for its reflection back to the channel  $i$ . To provide charge conservation, the net particle flux in the channels connecting the system with the reservoir must be zero. So we have:

$$J_3 + J_4 - J'_3 - J'_4 = 0. \quad (5)$$

The transmission function  $T(E)$  relates the particle flux outgoing from the channel 2 to the flux incoming to the channel 1, namely:

$$J'_2 = T(E) J_1. \quad (6)$$

Using Eqs. (4) and (5) we can express the transmission function in terms of the matrix elements of the scattering matrix  $S$  relating the outgoing wave amplitudes  $b'_1, b'_2, a'_3, a'_4$  to the incident ones  $b_1, b_2, a_3, a_4$ :  $T_{ij} = |S_{ij}|^2$ . In the considered case of a single site bridge the  $S$  matrix takes the form [14]:

$$S = Z^{-1} \begin{pmatrix} r_1 + \alpha^2 r_2 & \alpha t_1 t_2 & \beta t_1 & \alpha \beta t_1 r_2 \\ \alpha t_1 t_2 & r_2 + \alpha^2 r_1 & \alpha \beta r_1 t_2 & \beta t_2 \\ \beta t_1 & \alpha \beta r_1 t_2 & \beta^2 r_1 & \alpha r_1 r_2 - \alpha \\ \alpha \beta t_1 r_2 & \beta t_2 & \alpha r_1 r_2 - \alpha & \beta^2 r_2 \end{pmatrix}. \quad (7)$$

where  $Z = 1 - \alpha^2 r_1 r_2$ ,  $\alpha = \sqrt{1 - \epsilon}$ ,  $\beta = \sqrt{\epsilon}$ ,  $r_{1,2}$  and  $t_{1,2}$  are the amplitude transmission and reflection coefficients for the barriers ( $|t_{1,2}|^2 + |r_{1,2}|^2 = 1$ ), and the parameter  $\epsilon$  characterizes the dephasing strength. This parameter takes values within the range  $[0, 1]$ , so that  $\epsilon = 0$  corresponds to the completely coherent and  $\epsilon = 1$  to the fully incoherent transport.

When the bridge is detached from the dephasing reservoir  $T(E) = |S_{12}|^2$ . On the other hand, in this case we

can employ a simple analytical expression for the electron transmission function [26, 27, 28]

$$T(E) = 4\Delta_1(E)\Delta_2(E)|G(E)|^2, \quad (8)$$

where  $\Delta_{1,2}(E) = -\text{Im}\Sigma_{1,2}(E)$ . In this expression, self-energy terms  $\Sigma_{1,2}$  appear due to the coupling of the metallic grains to the intermediate state (the bridge). The retarded Green's function for a single-site bridge could be approximation as follows:

$$G(E) = \frac{1}{E - E_1 + i\Gamma} \quad (9)$$

where  $E_1$  is the site energy. The width of the resonance level between the grains is described by the parameter  $\Gamma = \Delta_1 + \Delta_2 + \Gamma_{en}$  ( $\Gamma_{en}$  describes the effect of the environment).

Equating the expression (8) and  $t_1^2 t_2^2$  we arrive at the following expressions for the tunneling parameters  $\delta_{1,2}(E)$ :

$$\delta_{1,2}(E) \equiv t_{1,2}^2 = \frac{2\Delta_{1,2}}{\sqrt{(E - E_1)^2 + \Gamma^2}}. \quad (10)$$

Using this result we easily derive the general expression for the electron transmission function:

$$T(E) = \frac{g(E)(1 + \alpha^2)[g(E)(1 + \alpha^2) + 1 - \alpha^2]}{[g(E)(1 - \alpha^2) + 1 + \alpha^2]^2} \quad (11)$$

where:

$$g(E) = 2\sqrt{\frac{\Delta_1\Delta_2}{(E - E_1)^2 + \Gamma^2}}, \quad (12)$$

In studying the effect of the stochastic nuclear motions (effect of the temperature) on the intergrain electron transport we may treat the former as a phonon bath. In the present work we assume that the intermediate site (the bridge) is directly coupled to the phonons produced by nuclear motions. Such approach was used before in some papers analyzing dissipative effects in the electron conduction through molecules (see e.g. [15]), and we apply it here. Then  $\Gamma_{en}$  equals  $\Gamma_{ph}$  where  $\Gamma_{ph}(E)$  is the imaginary part of the electronic self-energy correction due to the electron-phonon interaction. However, in analyzing the electron transport in polymers, as well as in molecules, one must keep in mind that besides the bridge sites there always exist other nearby sites. In some cases the presence of such sites may strongly influence the effects of the stochastic nuclear motions on the characteristics of the electron transport. This may happen when the nearby sites somehow “screen” the bridge sites from the direct interaction with the phonon bath [17]. We elucidate some effects which could appear in the electron transport in conducting polymer fibers in the case of such indirect coupling of the bridge state to the phonon bath elsewhere [29].

To achieve better understanding of the effect of temperature in the electron transport in polymer fibers within the adopted approach we must express the dephasing strength  $\epsilon$  in terms of relevant energies. As shown before (see [30]),  $\epsilon$  could be written in the form:

$$\epsilon = \frac{\Gamma_{ph}}{\Gamma}. \quad (13)$$

In further calculations we assume that the phonon bath is characterized by the continuous spectral density  $J(\omega)$  of the form [31]:

$$J(\omega) = J_0 \frac{\omega}{\omega_c} \exp\left(-\frac{\omega}{\omega_c}\right) \quad (14)$$

where  $J_0$  describes the electron-phonon coupling strength, and  $\omega_c$  is the cut-off frequency of the bath characterizing the thermal relaxation rate of the latter.

Starting from the corresponding result of the earlier works [15, 27, 28] and using this expression 14 we may present  $\Gamma_{ph}(E)$  as follows:

$$\begin{aligned} \Gamma_{ph} = & 2\pi J_0 \int d\omega \frac{\omega}{\omega_c} \exp\left(-\frac{\omega}{\omega_c}\right) \\ & \times \{N(\omega)[\rho_{el}(E - \hbar\omega) + \rho_{el}(E + \hbar\omega)] \\ & + [1 - n(E - \hbar\omega)]\rho_{el}(E - \hbar\omega) \\ & + n(E + \hbar\omega)\rho_{el}(E + \hbar\omega)\}. \end{aligned} \quad (15)$$

Here,

$$n(E) = \frac{\Delta_1 f_1(E) + \Delta_2 f_2(E)}{\Delta_1 + \Delta_2} \quad (16)$$

$\rho_{el}(E) = (-1/\pi)\text{Im}(E - E_1 + i\Gamma)^{-1}$  is the electron density of states,  $N(\omega)$  is the Bose-Einstein distribution function for the phonons at the temperature  $T$ . The asymptotic expression for the self-energy term  $\Gamma_{ph}$  depends on the relation between two characteristic energies, namely:  $\hbar\omega_c$  and  $kT$  ( $k$  is the Boltzmann constant). At moderately high temperatures ( $T \sim 100 \div 300K$ ), which are typical for the experiments on electrical characterization of polymer nanofibers  $kT \sim 10 \div 30meV$ . This is significantly greater than typical values of  $\hbar\omega_c$  ( $\hbar\omega_c \sim 1meV$  [15]). Therefore in further calculations we assume  $\hbar\omega_c \ll kT$ . Under this assumption, the main contribution to the integral over  $\omega$  in the Eq. (15) originates from the region where  $\omega \ll \omega_c \ll kT/\hbar$ , and we can use the following approximation:

$$\Gamma_{ph}(E) = \frac{2\Gamma\Lambda(J_0, \omega_c, T)}{(E - E_1)^2 + \Gamma^2}. \quad (17)$$

Here,

$$\Lambda = \frac{4J_0}{\hbar\omega_c} (kT)^2 \zeta\left(2; \frac{kT}{\hbar\omega_c} + 1\right) \quad (18)$$

where  $\zeta(2; kT/\hbar\omega_c + 1)$  is the Riemann  $\zeta$  function:

$$\zeta = (2; kT/\hbar\omega_c + 1) = \sum_{n=1}^{\infty} \frac{1}{(n + kT/\hbar\omega_c)^2}. \quad (19)$$

Under  $\hbar\omega_c \ll kT$ , we may apply the estimation  $\Lambda \approx 4kTJ_0$ .

Solving the equation (17) we obtain a reasonable asymptotic expression for  $\Gamma_{ph}$ :

$$\Gamma_{ph} = \frac{\Delta_1 + \Delta_2}{2} \frac{\rho^2(1 + \sqrt{1 + \rho^2})}{4\left(\frac{E - E_1}{\Delta_1 + \Delta_2}\right)^2 + (1 + \sqrt{1 + \rho^2})^2}. \quad (20)$$

where  $\rho^2 = 8\Lambda/(\Delta_1 + \Delta_2)^2$ . Substituting this expression into (13) we arrive at the result for the dephasing strength  $\epsilon$ :

$$\epsilon = \frac{1}{2} \frac{\rho^2(1 + \sqrt{1 + \rho^2})}{4\left(\frac{E - E_1}{\Delta_1 + \Delta_2}\right)^2 + \frac{1}{2}(1 + \sqrt{1 + \rho^2})^3} \quad (21)$$

This expression shows how the dephasing parameter depends on the temperature  $T$ , the electron-phonon coupling strength  $J_0$ , and the energy  $E$ . In particular, it follows from the Eq. (21) that  $\epsilon$  reaches its maximum at  $E = E_1$ , and the peak value of this parameter is given by:

$$\epsilon_{max} = \frac{\sqrt{1 + \rho^2} - 1}{\sqrt{1 + \rho^2} + 1}. \quad (22)$$

The obtained result enables us to analyze the temperature dependencies of the electric current and conductance of the doped polymer fibers assuming that the resonance tunneling predominates in the intergrain electron transport in the absence of phonons.

### III. DISCUSSION

The maximum value of the dephasing strength is determined with two parameters, namely,  $T$  and  $J_0$ . As illustrated in the Fig. 2,  $\epsilon_{max}$  increases when the temperature rises, and it takes on greater values when the electron-phonon interaction is getting stronger. This result has a clear physical sense. Also, as follows from the Eq. 21, the dephasing parameter exhibit a peak at  $E = E_1$  whose shape is determined by the product  $kTJ_0$ . When either  $J_0$  or  $T$  or both enhance, the peak becomes higher and its width increases. The manifested energy dependence of the dephasing strength allows us to resolve a difficulty occurring when the inelastic contribution to the electron transmission function is estimated using the simplified approximation of the parameter  $\epsilon$  as a constant. Within such approximation, a significant rate of phase randomization appears in the electron transport between the metallic-like islands when

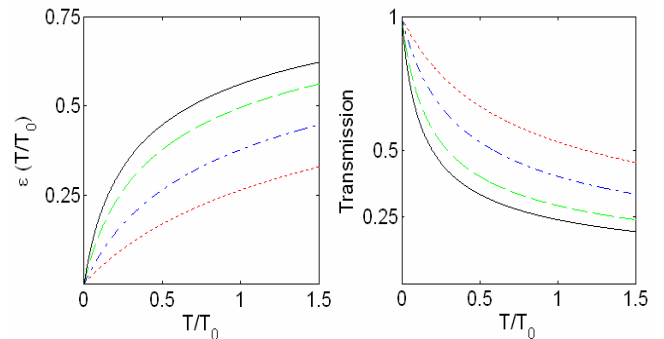


FIG. 2: Temperature dependencies of the the dephasing parameter  $\epsilon$  (left panel) and the electron transmission  $T$  (right panel). The curves are plotted at  $T_0 = 50K$ ,  $\Delta_1 = \Delta_2 = 4meV$ ,  $E = E_1 = 0$ ,  $J_0 = 9.0meV$  (solid line),  $6.0meV$  (dashed line),  $3meV$  (dash-dotted line),  $1.5meV$  (dotted line).

$\epsilon$  reaches values  $\sim 0.3 \div 0.5$  or greater [30]. Then the peak at the electron transmission is eroded, and current-voltage characteristics become linear. Therefore, to keep in consideration a distinguishable coherent contribution to the current, one must assume  $\epsilon$  to take on small values. For instance, the agreement with the experimental data reported in the work [18] was achieved assuming  $\epsilon = 0.05$  [32]. When the experiments are carried out at room temperatures such small values of  $\epsilon$  imply very weak electron-phonon coupling strength. This implication could hardly be given a reasonable physical explanation. On the contrary, if the energy dependence of  $\epsilon$  is accounted for, the peak in the electron transmission at  $E = E_1$  may be still distinguishable at moderately high values of the electron-phonon coupling strength  $J_0$ .

Current-voltage characteristics and voltage dependencies of the conductance  $G = dI/dV$  computed using the expressions 2, 11, 21 are presented in the Fig. 3. We see that as the electron-phonon coupling strengthens, the I-V curves lose their specific shape typical for the coherent tunneling through the intermediate state. They become closer to straight lines corresponding to the Ohmic law. At the same time the maximum in the conductance originating from the intergrain tunneling gets eroded due to the effect of phonons. These are the obvious results discussed in some earlier works (see e.g. [14]). The relative strength of the electron-phonon interaction is determined by the ratio of the electron-phonon coupling constant  $J_0$  and the self-energy terms describing the coupling of the intermediate state (bridge) to the leads  $\Delta_{1,2}$ . The effect of phonons on the electron transport becomes significant when  $J_0 > \Delta_{1,2}$ .

Otherwise, the coherent tunneling between the metallic-like islands prevails in the intergrain electron

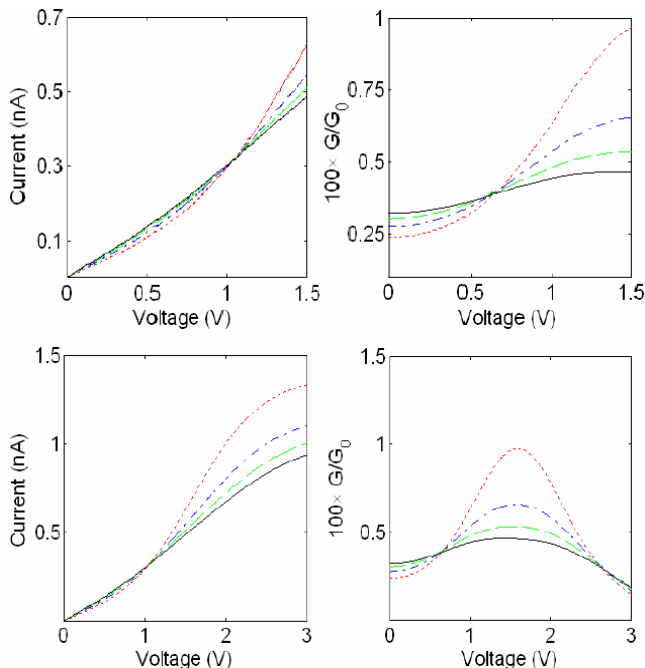


FIG. 3: Current (left panels) and conductance (right panels) versus voltage. The curves are plotted at  $T = 50K$ ,  $T = 30K$ ,  $E_1 = 40meV$ ,  $\Delta_1 = \Delta_2 = 4meV$ ,  $n = 1$ ,  $\Delta V/V = 0.005$ , assuming  $J_0 = 9meV$  (solid line),  $J_0 = 6meV$  (dashed line),  $J_0 = 3meV$  (dash-dotted line), and  $J_0 = 1.5meV$  (dotted line).  $G_0 = 2e^2/h$  is the quantum conductance.

transport, and the influence of thermal phonon bath is weak. Again, we may remark that  $J_0$  and  $T$  are combined as  $kTJ_0$  in the expression (21) for the dephasing strength  $\epsilon$ . Therefore an increase in temperature at a fixed electron-phonon coupling strength enhances the incoherent contribution to the current in the same way as the previously discussed increase in the electron-phonon coupling. Also, at low values of the applied voltage the electron-phonon coupling brings an enhancement in both current and conductance, as shown in the top panels of the Fig. 3, whereas the effect becomes reversed as the voltage grows above a certain value (see Fig. 3, the bottom panels). This happens because the phonon induced broadening of the intermediate energy level (the bridge) assists the electron transport at small bias voltage. As the voltage rises, this effect is surpassed by the scattering effect of phonons which resists the electron transport.

Now, we consider temperature dependencies of the electric current and conductance resulting from the intergrain electron tunneling via the intermediate localized state. These dependencies are shown in the Fig. 4. The curves in the figure are plotted at low bias volt-

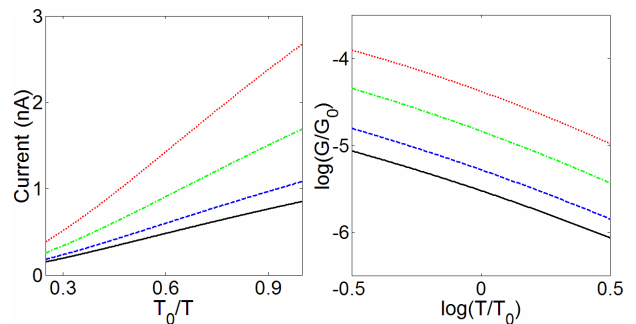


FIG. 4: Temperature dependence of current (left panel) and conductance (right panel) at low voltage bias ( $V = 0.3V$ ). The curves are plotted at  $T_0 = 50K$ ,  $J_0 = 9meV$  (solid line),  $J_0 = 6meV$  (dashed line),  $J_0 = 3meV$  (dash-dotted line), and  $J_0 = 1.5meV$  (dotted line). The values of remaining parameters coincide with those used in the figure 3.

age ( $V = 0.3V$ ,  $\Delta V/V = 0.005$ ) and  $T_0 = 50K$ , so  $e\Delta V < kT$ . This regime is chosen to compare the obtained temperature dependencies with those typical for the phonon assisted hopping transport discussed in the beginning of the present work. We see that the tunneling current temperature dependence shown in the left panel of Fig. 4 crucially disagrees with the Mott's expression describing the “hopping” electron transport. The tunnel current decreases as temperature rises being proportional to  $(T_0/T)^\beta$ , and the exponent  $\beta$  takes on values close to unity.

Already it was mentioned that the drop in the conductivity upon heating a sample was observed in polymers and carbon nanotubes. However, such metallic-like behavior could originate from various dc transport mechanisms. Correspondingly, the specific features of temperature dependencies of the conductivity and/or current vary depending on the responsible conduction mechanisms [33]. The particular temperature dependence of the electron tunneling current obtained in the present work and shown in the figure 3 differs from those occurring due to other transport mechanisms. Such dependence was observed in the experiment on the electron transport in a single low-defect-content carbon nanotube rope whose metallic-like conductivity was manifested within a wide temperature range ( $T \sim 35 \div 300K$ ), as reported by Fisher et al [34]. The conductivity temperature dependence observed in this work could be approximated as  $\sigma(T)/\sigma(300) \sim a + bT_0/T$  where  $A, b$  are dimensionless constants. The approximation includes the temperature independent term which corresponds to the Drude conductivity. The second term is inversely proportional to the temperature in agreement with present results for the current shown in the Fig. 3. It is also likely that a similar approximation may be adopted to de-



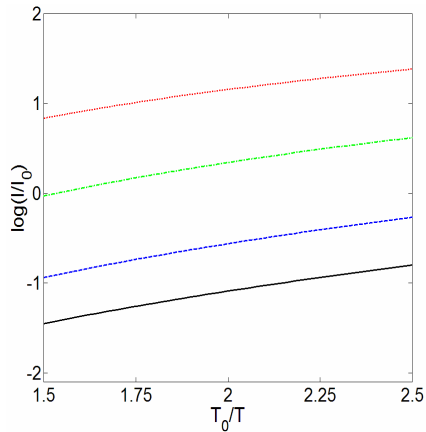


FIG. 5: Temperature dependence of the electron current at higher bias voltage ( $V = 2V$ ). The curves are plotted at  $T_0 = 50K$ ,  $J_0 = 9meV$  (solid line),  $J_0 = 6meV$  (dashed line),  $J_0 = 3meV$  (dash-dotted line), and  $J_0 = 1.5meV$  (dotted line). The values of remaining parameters are the same in the figures 3,4. The current  $I_0$  is computed using  $J_0 = 3meV$ ;  $T_0/T = 1.5$ .

scribe the experimental data obtained for chlorate-doped polyacetylene samples at the temperatures below  $100K$  [35]. In both cases we may attribute the contribution proportional to  $1/T$  to the resonance electron tunneling transport mechanism.

Also, the conductance due to the electron intergrain tunneling reduces when the temperature increases, as shown in the right panel of the Fig. 4. Irrespective of the electron-phonon coupling strength we may approximate the conductance by the power law  $G \sim T^\alpha$  where  $\alpha$  takes on values close to  $-1$ . This agrees with the results for the current. At higher bias voltage the temperature dependence of the current changes, as shown in the Fig. 5. The curves shown in this figure could be approximated as  $\ln(I/I_0) \sim c + dT_0/T$ ;  $c, d$  being dimensionless constants. This resembles typical temperature dependencies of the tunneling current in quasi-one-dimensional metals which were predicted for conducting polymers being in a metal state (see e.g. Ref. [2]).

Finally, there exist several mechanisms which could simultaneously work providing the charge transport in highly disordered and inhomogeneous materials as conducting polymers and their relative significance could vary depending on both specific intrinsic characteristics of particular materials (such as crystallization rate and electron-electron and electron-phonon coupling strengths) and on the external factors such as temperature. Various conduction mechanisms give rise to various temperature dependencies of the electric current and conductance which could be observed in polymer nanofibers/nanotubes. In the present work we carried

out theoretical studies to find out the character of temperature dependencies of both current and conductance provided by specific transport mechanism, namely, resonance tunneling of electrons.

Accordingly, we treat a conducting polymer as a kind of granular metal, and we assume that the intergrain conduction occurs due to the electron tunneling between the metalliclike grains through the intermediate state. To take into account the effect of temperature we represent the thermal environment (stochastic nuclear motions) as a phonon bath, and we introduce the coupling of the intermediate site to the thermal phonons. In calculations of the electron transmission in the presence of dissipation originating from the thermal environment we follow the way proposed in the work [30]. The latter is based on the Buttiker model within the scattering matrix formalism but instead of treating the dephasing strength as a phenomenological parameter, the latter is expressed in terms of relevant energies, such as temperature and electron-phonon coupling strength.

Using this approach we showed that the above described transport mechanism results in the temperature dependencies of transport characteristics which differ from those obtained for other conduction mechanisms such as phonon-assisted hopping between localised states. Being observed in experiments on realistic polymer nanofibers, the predicted dependencies would give grounds to suggest the electron tunneling to predominate in the intergrain electron transport in these particular nanofibers. We believe the present studies to contribute to better understanding of electron transport mechanisms in conducting polymers and carbon nanotubes. Also, we believe that the model developed here may be used to theoretically analyze inelastic electron transport through molecular junctions and nanodevices including quantum dots coupled to the electron reservoirs.

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